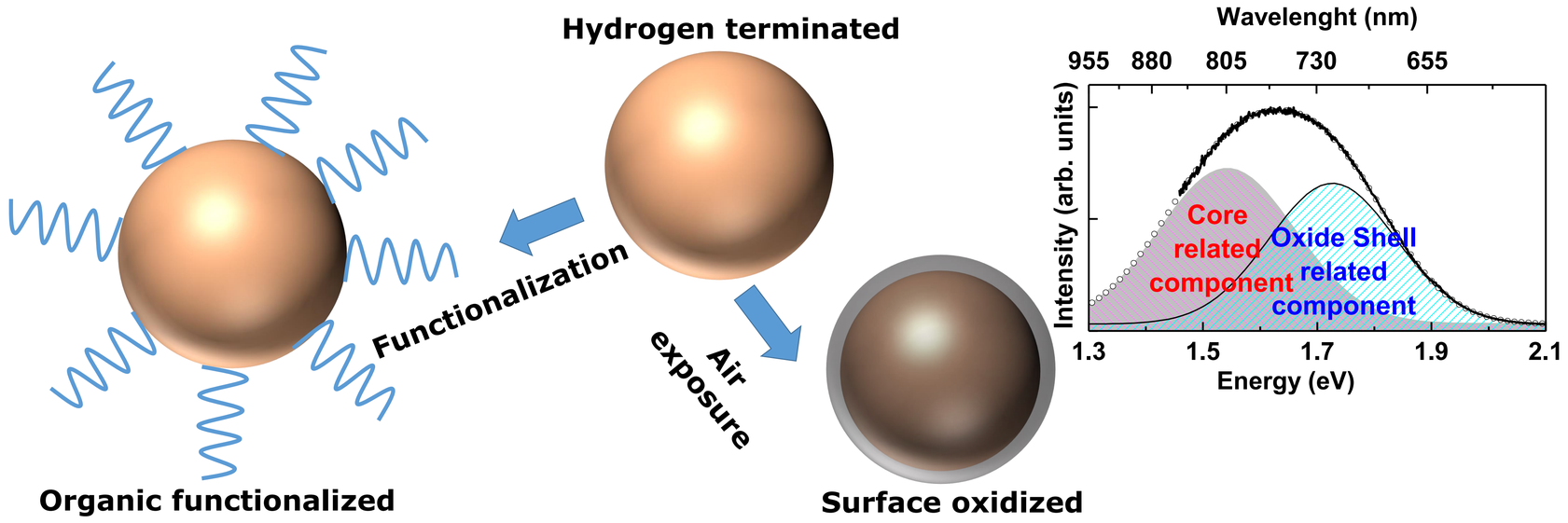
Core-shell and Core-host Interaction Effects on the Optoelectronic Properties of Functional Silicon Nanoparticles



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Objectives

Crystalline silicon nanoparticles (SiNPs) are currently under intense investigation due to their unusual and size-specific optical and electronic behavior. High quality of freestanding SiNPs can be produced using plasma-assisted decomposition of silanes (Figure 1) [1]. The step from isolated NPs to functional NPs raises novel questions regarding their sensitivity to the shell and surrounding environment.

The work aims at understanding the influence of external environment on the optoelectronic properties of crystalline silicon nanoparticles (SiNPs). Considering that light emission is affected by energy transfer across the core-shell and core-host, the spectroscopy becomes a privileged tool to study the optoelectronic properties.

Methods and techniques

Detailed spectroscopic analysis:

- Photoluminescence characterization (emission and excitation) in steady state and time-resolved (in the micro and nano second scale) modes in the temperature range between 10 and 350 K.
- Emission decay curves as function of the temperature, monitoring and excitation wavelengths.
- Measurement of the emission quantum yield excited at distinct excitation wavelengths.

Results

The broad band emission of the SiNPs after natural oxidation is formed of two components with distinct lifetimes (Figure 2), that are originated from distinct recombination mechanisms, taking place simultaneously in the same sample [2]. The identification and measurement of the lifetime of each component were possible by using time-resolved spectroscopy and by choosing the measurement time window at which only one of the emission mechanisms is active. The experiments indicate that one of the emissions is due to recombination of photogenerated electrons and holes located in the crystalline core of the SiNPs and the other is originated from donor-acceptor recombination pairs involving states associated with the native oxide shell [2].

The dependence of the emission quantum yield values on the surface termination (Figure 3) suggests that the probability of excitons migration between SiNPs, that reduce the efficiency of the light emission, is strongly affected by the surface ligands.

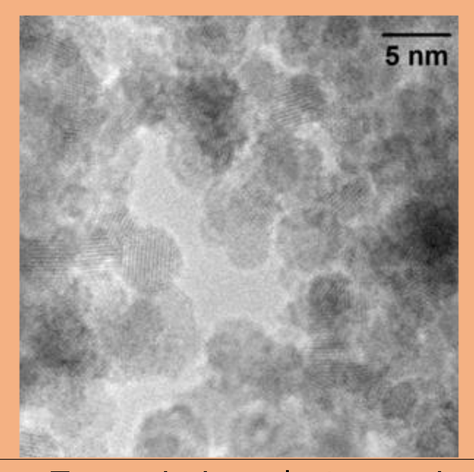

FIG. 1 – Transmission electron microscopy of hydrogen terminated SiNPs, produced by plasma-assisted decomposition of silane.

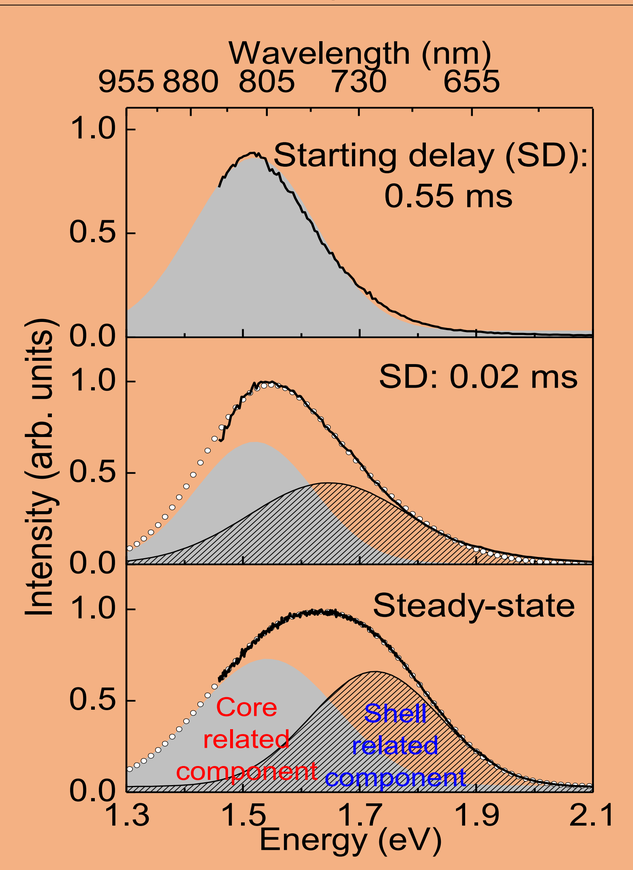

FIG. 2 – Low-temperature (12 K) time-resolved emission spectra of surface oxidized SiNPs excited at 365 nm at SD values of 0.55 and 0.02 ms, together with steady-state emission spectrum excited at 275 nm.

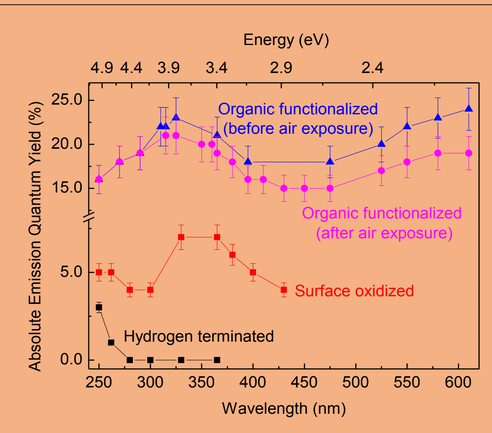

FIG. 3 – Absolute emission quantum yield values as function of the excitation wavelength for SiNPs with different surface terminations (processed as a film).

Publications

[1] Pereira, R. N., Rowe, D. J., Anthony, R. J. & Kortshagen, U. Freestanding silicon nanocrystals with extremely low defect content. *Phys. Rev. B* **83**, 085449-1-085449-6 (2012)

[2] Botas, A. M. P., Ferreira, R. A. S., Pereira, R. N., Anthony, R. J., Moura, T., Rowe, D. J. & Kortshagen, U. High Quantum Yield Dual Emission from Gas-Phase Grown Crystalline Si Nanoparticles. *J. Phys. Chem. C* **118**, 10375-10383 (2014)

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